Comparison Between the Experimentally Determined Orientation Dependence of the Near Edge Structure in Electron Energy Loss Spectra from Graphite with Present Theoretical Formulations.

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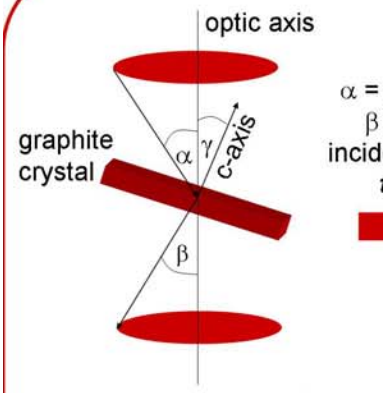
Motivation.

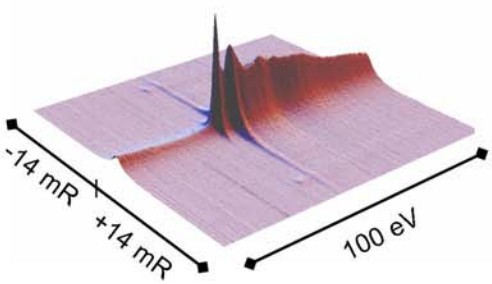
Electron Energy Loss Spectroscopy (EELS) in the Transmission Electron Microscope (TEM) is the technique of choice for the spatially resolved chemical fingerprinting of amorphous carbon compounds. In this process crystalline graphite is generally used as the sp^2 standard. However, the Energy Loss Near Edge Structure (ELNES) from graphite is highly orientation dependent, making its comparison with amorphous materials difficult. Many works prescribe a set of experimental conditions that minimise the orientation dependence, i.e. the "magic angle". Not only does this throw away valuable resolution, but there are many discrepancies both between theories, and between experiments. New measurements using high angular resolution electron channeling electron spectroscopy (HARECES) from the graphite K edge are mined to compare to theoretical predictions.

Experiment.



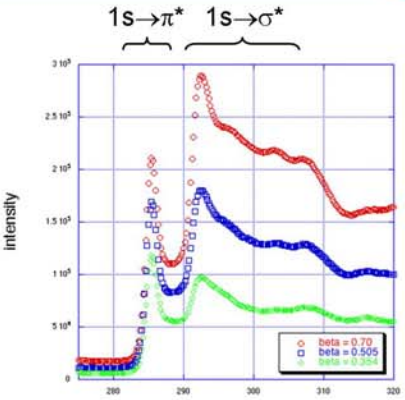
α = convergence semi-angle
β = collection semi-angle

α = 0, γ = 0, β small, incident beam ***tilted***



Angularly resolved energy loss surface.

integrate data to examine variation with β

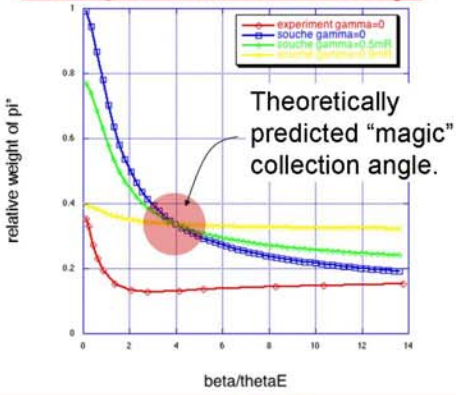


Variation in K-Edge Profile with β

Comparison to Theory.

The relative weight of the π* contribution can be determined from the spectra and directly compared to theoretical predictions (e.g. C. Souche, B. Jouffrey, G. Hug and M. Nelhiebel. ***Micron***, **29**, 419-424, (1998).)

$$\text{rel. weight of } \pi^* \text{ (expt.)} = \frac{N(1s \rightarrow \pi^*)}{N(1s \rightarrow \pi^*) + N(1s \rightarrow \sigma^*)}$$



The general shape of the theoretical curves match the data, but close inspection shows the two are not linear at the large collection angles generally used for experiment.
The theoretical value of the relative weight of the π* contribution drops off monotonically with collection angle, but there is a shoulder in the data which may evidence a physical effect that is unaccounted for in the theory.

Major Conclusions.

HARECES data from the graphite K edge provides a versatile and continuous data set which may be mined for close comparison with theory. Early work indicates that some effect, such as electron channeling, may be unaccounted for in the theory.

Future Directions.

The refinement of present theories describing the orientation dependence of the ELNES of the graphite K edge will permit vast improvements in the chemical fingerprinting of amorphous carbon compounds with EELS.

N. J. Zaluzec, M. G. Blackford, K. L. Smith and M. Colella, Microscopy and Microanalysis Vol 11, Sup. 2, 718, (2005).

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